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AI in Drug Development Series: Takeaways From Our Call With Insilico Medicine

We hosted the CEO of Insilico Medicine, Alex Zhavoronkov, for a conversation on the role of AI in drug discovery. He highlighted faster early discovery, limited value of proprietary data, and balancing target novelty vs validation.

We hosted an AI in drug discovery (AIDD) webcast with Insilico Medicine CEO Alex Zhavoronkov (publicly listed in Hong Kong and covered by Jack Lin), which offered a pragmatic reframing of AI's role across drug discovery. While earlier industry narratives emphasized wholesale disruption, management now highlights that AI's impact is most tangible in accelerating and de-risking early discovery workflows rather than replacing core scientific functions. Insilico progressed 13 internally developed programs into the clinic (including three Phase 2 assets), underscoring its position as one of the more clinically validated AIDD platforms.

The CEO opined on the limited durability of proprietary datasets as a competitive moat in AIDD. Despite maintaining a large internally generated dataset—including >3,000 disease-target associations—the CEO argued that access to differentiated data alone has not translated into drug development success industrywide, highlighting a “graveyard” of data-centric companies that failed to deliver. Instead, he emphasized integrated benchmarking systems—Insilico maintains ~1.2K proprietary benchmarks—and model orchestration as more meaningful differentiators with performance ultimately constrained by broader industry limitations such as translatability of animal models and availability of disease-relevant assays.

Organoids and other non-human alternatives may not replace animal studies in the near term. Alex emphasized that the real bottleneck for AIDD is not safety validation, which may be partially replaceable, but rather the lack of efficacy for models in reliably translating to human disease. While safety testing can be improved through robotic labs, organoids, and existing primate data, companies cannot fully eliminate animal testing due to limited regulatory acceptance of fully animal-free validation packages. The larger challenge remains efficacy, especially in chronic and age-related diseases such as Alzheimer's, Parkinson's, ALS, and fibrosis, where short-lived mice or monkeys cannot naturally replicate long-cycle human pathology. Thus, current models often rely on artificial induction methods which have limited biological correlation with spontaneous human disease and limit their regulatory alignment without animal testing.

On commercialization, management stressed that achieving economic viability in AIDD requires thoughtful tradeoffs between target novelty and validation. While

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novel targets may command higher theoretical value, they typically require significant clinical de-risking (often through Phase 2) before attracting meaningful partner interest resulting in higher capital intensity and longer timelines. In contrast, programs against more validated targets, paired with improved molecular design, are more readily monetizable at earlier stages. Insilico's strategy has therefore shifted toward balancing novelty across target and chemistry to optimize out-licensing opportunities and drive a path toward profitability.

Finally, the discussion reinforced that AIDD's most validated benefit today lies in compressing early discovery timelines and reducing cost to preclinical candidate (PCC), rather than fundamentally altering clinical development timelines. Insilico cited ~12–18 months and ~\$3–5mn to reach PCC, with continued improvements in computational efficiency (from weeks to days). However, downstream development remains bounded by regulatory and biological constraints, with no meaningful acceleration expected in IND-enabling or clinical phases. Taken together, AIDD appears best positioned today as a productivity-enhancing layer within drug discovery, particularly in hit-to-lead and lead optimization, rather than a step-change disruptor of the broader R&D paradigm.

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Underweight/Sell	555	15%	84	9%	15%	202	12%
Total	3,673		909			1627	

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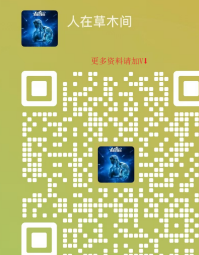
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